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# Cryogenic, Multiphase, Hydrogen-Oxygen Detonations

Edward B. Coy<sup>\*</sup> and Jonathan M. Watts<sup>†</sup>  
*Air Force Research Laboratory, Edwards AFB, CA 93524*

Sampath Palaniswamy<sup>‡</sup>  
*Metacomp Technologies, Agoura Hills, CA*

**Detonations of flowing mixtures of hydrogen and oxygen at temperatures between 90 and 110 K, pressures from 3 to 5 bar, and mixture densities of 3-6 kg/m<sup>3</sup> have been studied. The effect of liquid oxygen on wave speeds and peak wall pressures are reported. Data taken at cryogenic conditions are compared with ambient temperature data taken at similar initial densities and equivalence ratios, as well as with equilibrium, Chapman-Jouget theory calculations. For the conditions studied, liquid oxygen was found to result in increased wave speeds and peak wall pressures. These observations are shown to be consistent with a highly stratified mixture with high concentrations of oxygen in a layer adjacent to the wall and low concentrations along the axis of the tube.**

## I. Introduction

**T**HIS paper presents results from an investigation of detonations of flowing mixtures of cryogenic gaseous hydrogen and liquid oxygen. This work was undertaken to support development of pulse detonation rocket engines (PDRE). Cryogenic propellants will be desirable for PDRE applications for many of the same reasons that they are used for conventional rocket engines: the density is increased, which reduces tank volume, and cooling of the combustion chamber is facilitated. There is an additional advantage for PDREs insofar as a major advantage of the cycle is the reduced pumping requirements associated with the low injection pressures. High density enables a larger mass to be charged into the chamber for a given supply pressure. Hydrogen and oxygen were chosen for this study due to their high specific impulse, ease of detonability, and the existing experience with handling and design.

There is an extensive list of phenomena which could be significant in detonations of liquid oxygen and hydrogen. There are phenomena that affect the initial state of the mixture which include atomization, turbulent dispersion, vaporization, turbulent mixing, wall-wetting, and heat-transfer. Other phenomena affect the propagation of the detonation through the mixture which include droplet shattering, vaporization, chemical induction time, wall friction and heat transfer within the reaction zone, and longitudinal and axial variations in the mixture composition. There have not been any previous studies which characterized the propagation of detonations under all of these complex conditions. Studies which examined subsets of the problem are briefly reviewed here.

Previous studies of detonations of cryogenic, quiescent, gaseous mixtures of hydrogen and oxygen have found that measured wave velocities and pressures agree well with ideal-gas equilibrium Chapman-Jouget calculations up to initial pressures of approximately 5 atm and densities of 5 kg/m<sup>3</sup>.<sup>1,2,3</sup> At higher pressures and densities the ideal-gas calculations under-predict wave speed and pressure, and a real-gas equation of state produces better agreement. This result was also obtained in a study of ambient temperature, high-pressure (up to 40 atm) quiescent, hydrogen-oxygen detonations.<sup>4</sup>

There are an extensive number of references on detonations in sprays. The vapor pressure of the fuel has a large influence on the propagation mechanisms of the detonation. For high vapor pressure liquids, a detonation can be supported in the gas-phase, and the liquid fraction is consumed in the products and does not contribute to the processes which drive the leading shock. For low vapor pressure liquids, the successful propagation of a detonation has been shown to depend on the rate at which droplets are decomposed into a "micromist" by the high velocity

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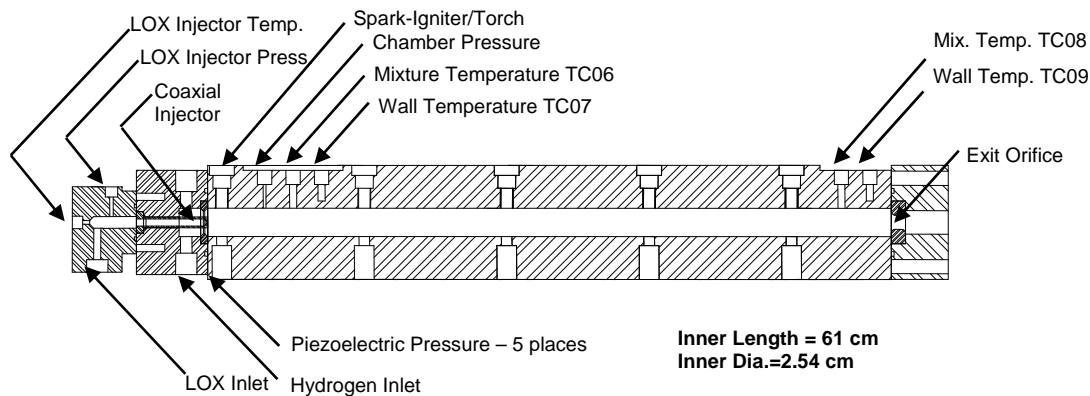
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<sup>\*</sup> Propulsion Research Engineer, Aerophysics Branch, 10 East Saturn Blvd., Member AIAA

<sup>†</sup> Propulsion Research Engineer, Aerophysics Branch, 10 East Saturn Blvd.

<sup>‡</sup> Senior Scientist, Metacomp Technologies, Member AIAA



**Figure 1. Cross-section view of test article showing locations of instrumentation. Orientation was vertical during tests.**

flow following the leading shock wave<sup>5</sup>. Studies using 400-2600 micron droplets have shown that following a chemical induction time delay, the micromist explodes, sending shock waves forward to reinforce the leading shock, and rearward, as a retonation. The droplet shattering and evaporation processes are much slower than the gas-phase kinetics of the combustion reactions and result in much longer reaction zones than are typical of gas phase detonations. It has also been observed that a thin film of a low vapor-pressure liquid hydrocarbon deposited on the wall of a tube can support a combustion wave that propagates at nearly the CJ velocity<sup>6</sup>. In this case the high-velocity gas behind the leading shock creates a shear flow over the liquid that strips away small droplets. The droplets rapidly react, and the heat release sustains the process.

Due to their fundamentally different mode of propagation, low vapor pressure spray and film detonations do not in general match propagation velocities and pressures obtained from CJ thermodynamic equilibrium calculations. Wave velocities and pressures are typically reduced. For detonations in tubes the discrepancy has been attributed to heat transfer and wall friction in the extended reaction zone<sup>5</sup>. For detonations initiated directly by high explosive charges, the discrepancy has been attributed to the simultaneous decay of the initiating blast wave and increasing length of the reaction zone, implying that the reduced velocity is a transient phenomena and that the theoretical value would be reached in a sufficiently long apparatus.<sup>7</sup>

The purpose of this work was to experimentally investigate the behavior of detonating mixtures of liquid oxygen and cryogenic gaseous hydrogen under conditions expected to be relevant to pulse detonation rocket engines. The results are applicable to the development of the next generation of repetitively pulsed, multi-tube test articles and also are intended to be used to qualify computational models under development for use in system application studies.

## II. Experimental Setup

The test article was a vertically oriented, 304 stainless steel tube, with 61 cm inner length and a 2.54 cm inner diameter and a design pressure of 70 MPa. The injector was a swirled co-axial design. Angular momentum was imparted to the liquid oxygen through an off-axis inlet port. Oxygen exited through the center post and hydrogen through the surrounding annulus. Visualization of the injector flow was performed using air and water as simulants in the AFRL/PRSA Flow Laboratory. Water matched the density and volumetric flow rate of liquid oxygen to within 5%. Atmospheric pressure air matched the density of hydrogen at the test conditions to within 10% and the volumetric flow rate within 5%. The liquid was well atomized with a maximum droplet size of approximately 100 micrometers. The injector produced a hollow-cone spray with a divergence angle of 30° resulting in the majority of the liquid being deposited on the walls of the tube during the experiments.

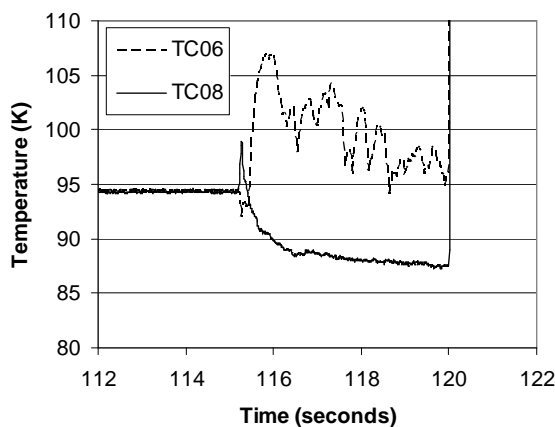
The fuel for the detonation tests was industrial grade hydrogen, 99.9% pure with methane as the principal impurity. The hydrogen was supplied from high-pressure cylinders and chilled to cryogenic temperatures in a shell-and-tube heat exchanger with saturated, 2.6 atm liquid nitrogen on the shell side. The hydrogen mass flow rate was measured using a sonic nozzle. The mass flow rate was calculated using an in-house developed program that solves the 1-D Euler equations for sonic orifice flow using real-gas properties. The discharge coefficient for the nozzle was provided by the manufacturer and was certified to be accurate within +/- 2%.

Industrial grade liquid oxygen, 99.5 % with nitrogen as the principal impurity, was supplied from a 200 liter dewar pressurized with helium. Volumetric flow rate was measured using a turbine meter, and the inlet state was measured with a thermocouple and pressure transducer to determine the density. The dewar was located on an electronic scale to enable the flow rate of liquid oxygen to be independently determined from the rate of change of mass of the dewar. This arrangement enabled the turbine meter to be calibrated in-situ with an accuracy of  $\pm 0.5\%$ .

The extent of vaporization of liquid oxygen varied along the length of the test article due to heat transfer to the oxygen from the hydrogen and the tube wall. Two methods were used to estimate the extent of vaporization. The first assumed adiabatic mixing of the streams of hydrogen and oxygen at the inlet enthalpies and is listed in the data tables below as the initial gaseous oxygen fraction. The second assumed that liquid and gas phases reached thermal equilibrium at the measured exit temperature. This assumption was supported by typical data for mixture temperature as shown in figure 2. Prior to 115 seconds both thermocouples were exposed to saturated oxygen at a pressure of 1.5 atm. At 115 seconds the hydrogen flow was initiated and a two-phase mixture of hydrogen and liquid oxygen began impinging on TC06 causing large fluctuations in temperature. The temperature trended downward as the flow from the heat exchanger cooled the system components and the hydrogen inlet temperature decreased. Near the exit at TC08 the hydrogen and oxygen had reached thermal equilibrium as evidenced by the lack of fluctuations. Based on the measured temperature at TC08 the vapor pressure of gaseous oxygen was determined from the saturation curve and this was used to determine the mass fraction of oxygen in the gas phase. For the case shown, the mass fraction of oxygen in the gas phase was  $0.76 \pm 0.08$ . In several cases the temperature fluctuations at TC08 indicated that thermal equilibrium had not been reached. For those cases the reported value of oxygen mass fraction was based on the average temperature, and the uncertainty was based on the magnitude of the temperature fluctuations. To complete the discussion of the figure, at 120 seconds the mixture was ignited and both thermocouples went off-scale.

All thermocouples were checked for accuracy in a liquid nitrogen bath prior to installation. In addition, during each test the interval when saturated oxygen was present enabled routine checks to be performed. To prevent the thermocouples exposed to the detonation products from melting, the beads were blanketed with a flow of nitrogen that was initiated coincident with the ignition.

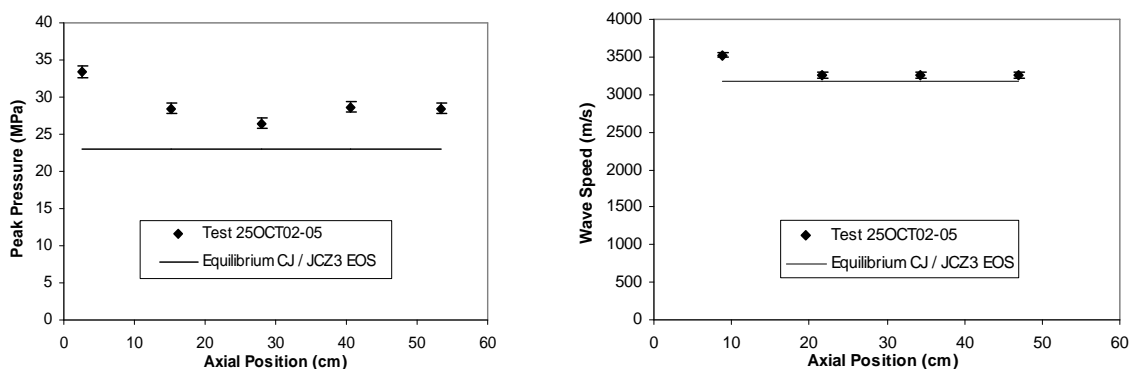
Five piezoelectric transducers (Kistler 603B1) were mounted flush with the inner surface of the tube at 12.7 cm intervals. The signals were recorded at 1 MHz and 12 bit resolution for a precision of 24 KPa. Each transducer, associated range capacitor (Kistler 571A3), impedance-converter (Kistler 558), and cables were calibrated as a set by the manufacturer and certified to be linear to less than  $\pm 1\%$  of full scale. The calibrations were performed at 295 K over the range 0-69 MPa. The manufacturer's literature listed a nominal value for the temperature coefficient of sensitivity of  $-0.027\%/K$ . For the cryogenic tests this amounted to  $-5.5\%$ ; however, because a calibration was not performed at the operating temperature, we have estimated the uncertainty at  $\pm 10\%$ . The response of the piezoelectric transducers was checked in our laboratory under shock tube and gaseous detonation conditions. For the shock tests, a driver tube and burst disc were installed in place of the injector, and the exit orifice was replaced with a blank. The measured wave speed was used to predict pressure behind the incident and reflected shocks using a thermodynamic equilibrium model. The predicted values agreed within 10% with the measurements. The gaseous detonation tests were performed with flowing mixtures. The flow rates were set to produce an initial density and equivalence ratio representative of the target conditions for the cryogenic tests. The measured peak pressures and wave speeds are shown in figures 3 and 4 for a test with an initial mixture density of  $3.6 \pm 0.1 \text{ Kg/m}^3$  and an equivalence ratio of  $1.5 \pm 0.1$ . The pressure signals were not filtered. The trends in pressure and velocity are consistent with an initially over-driven detonation relaxing to a steady state. Also given are equilibrium Chapman-Jouget calculations obtained using the Cheetah code<sup>8</sup> with 10 product species. The calculations were performed using ideal-gas and JCZ3 equations of state. The results differed by about 1% in both pressure and velocity with slightly better agreement obtained with JCZ3. These results are



**Figure 2. Mixture temperatures at inlet (TC06) and exit (TC08). Prior to 115 s saturated oxygen is flowing. At 115 s hydrogen flow is started. At 120 s ignition occurs. Liquid and gas have reached thermal**

included here to indicate the level of agreement with CJ theory that was obtained for ambient-temperature, gaseous detonations and will be compared with results presented below for cryogenic, liquid-gas detonations.

The spark ignition system was a conventional automotive system, and produced approximately 110 millijoules per spark. The spark plug was a surface gap, Champion G52V. When the spark plug was cooled below approximately 100 K it would not discharge, so it could not be located in the wall of the test article. An ignition chamber with a volume of approximately 15 cm<sup>3</sup> was added that could be maintained above 100 K with heating tape. Prior to ignition the chamber was charged from the hydrogen-oxygen mixture flowing in the test article, and at ignition it injected a flame jet into the test article through a 5 mm orifice. The ignition chamber could be located near the injector at the position shown in figure 1 or in the exhaust tube downstream of the exit orifice. The detonation velocities given in the figures are averages over the 12.7 cm intervals between transducers and were based on the time the pressure signals had risen to at least half of their peak value. The manufacturer's literature specifies that the Kistler 603B1 transducers have a rise time from 10-90% of 1  $\mu$ s. The signals were also digitized at 1  $\mu$ s intervals. Assuming the timing of the wave arrival could be in error by one microsecond, the uncertainty of wave speed ranged from +/- 65-110 m/s.



**Figures 3 and 4. Peak wall pressures and wave velocities from an ambient temperature detonation of a flowing mixture of hydrogen and oxygen. Equilibrium CJ calculations were performed using the Cheetah code and the JCZ3, real-gas, equation of state. Level of agreement between measurements and theory can be compared with results for cryogenic mixtures.**

### A. Experimental Methodology

Prior to a firing, the liquid oxygen dewar was vented to atmosphere and the oxygen was allowed to boil until it reached a saturated state. The propellant systems and test article were cooled with liquid nitrogen. When temperatures reached 100 K, the liquid oxygen dewar was pressurized with helium, and the systems were flushed and filled with propellants. The automated firing sequence began by flowing liquid oxygen until the fluid was sub-cooled by approximately 20 K at the injector. This typically required 60-120 seconds. The hydrogen flow began approximately 5 seconds before ignition. At 100 milliseconds prior to ignition, the test article and injector pressure transducers were isolated to prevent over-ranging. At the time of ignition, liquid oxygen temperatures at the injector were in the range of 95-115 K, hydrogen inlet temperatures were 100-120 K and wall temperatures were 110-120 K. Pressure in the test article was 2.7-4.4 atm. The spark system was fired, and a warm nitrogen purge flow was initiated to flush combustion products and minimize ice formation in the tube. Several series of tests were performed at fixed flow rates of hydrogen and varying flow rates of oxygen. At low oxygen flow rates the liquid was entirely vaporized, and at higher flow rates an increasing fraction remained a liquid.

## III. Results

The initial conditions for two representative tests at high equivalence ratio are given in table 1. Both tests had liquid oxygen present at the injector and were fully vaporized at the exit condition. In test 12FEB04-17 the mixture was ignited in the exhaust tube and the detonation propagated towards the injector. In test 18FEB04-03 the ignition was at the injector and the detonation propagated towards the exit orifice. Wave speeds and peak wall pressures are shown in figures 5 and 6. The arrows indicate the direction of propagation. The measured wave speeds agree

within 5% with the equilibrium code predictions except near the injector, where the measured velocity is significantly lower. The level of agreement away from the injector is similar to that obtained in the ambient temperature detonations at similar densities. The measured peak pressures are a factor of two or more higher than the equilibrium code predictions. This is a larger deviation than was observed in the ambient temperature detonations and is believed to be significant. The changes in pressure along the tube do not appear to be correlated with changes in wave speed. There also is no observable effect on pressures or wave speeds due to the ignition location.

Table 2 gives the initial conditions for two representative tests at near-stoichiometric equivalence ratio. The initial gaseous oxygen fractions are significantly lower than those in the high equivalence ratio tests due to the higher flow rate of liquid oxygen. The exit flow is predicted to be fully vaporized in both cases; however, inspection of the exit temperature time traces showed there were fluctuations indicating full thermal equilibrium had not been reached. Both tests exhibit wave speeds approximately 20% greater than the equilibrium code predictions, however, there were also cases where the wave speed nearly matched the equilibrium value or fell a few percent below. The high velocity cases are particularly noteworthy, because deviations of this magnitude have not been reported previously for cryogenic or spray detonations. The peak pressures are approximately a factor of two greater than the equilibrium code, and the fluctuations in pressure do not appear to be correlated to changes in wave speed. The ignition location did not have an observable effect.

A summary of the wave speed results plotted as a function of equivalence ratio is given in figure 13. The average velocity over the 50.8 cm interval between the first and last transducers is shown. The equilibrium CJ calculations were performed assuming a nominal initial density of  $4 \text{ kg/m}^3$  as wave speed is a weak function of the initial density. The CJ calculation stands as a lower bound on the data. This is a noteworthy result, as other studies of detonations in sprays have found that the equilibrium CJ velocity is an upper bound and only reached in the limit of very small droplets or high vapor pressure fuels. The data were examined to determine if wave speed was correlated with any other parameter such as the extent of vaporization of the oxygen, the density of the mixture, the direction of propagation, the peak pressure of the wave, the initial wall temperature, and the date of the test. The wave speed did not correlate with any of these variables.

A summary of the peak pressure data is given in figure 14. Pressure is a strong function of the initial density as well as the equivalence ratio, so the measured pressures were normalized by the equilibrium CJ values calculated for each test condition. The average value and the standard deviation for each measurement location are shown. The deviations of the averages from the CJ values are statistically significant for all except the first transducer and are greater than the  $\pm 10\%$  uncertainty that was assigned to the pressure measurement. The high peak wall pressures must therefore be a feature of the test conditions.

In addition to the average deviations from the CJ values, peak pressures also exhibited large changes within a given test. The average value of the coefficient of variation for the five measurements of peak pressure within each test was 29%. The COV for the variation from test to test ranged from 57% for the first transducer to 20% for the fourth. These measures are comparable in magnitude and greater than the uncertainty in the pressure measurement; therefore, large fluctuations in peak wall pressures as well as random deviations from the CJ value are features of the test conditions.

## IV. Discussion

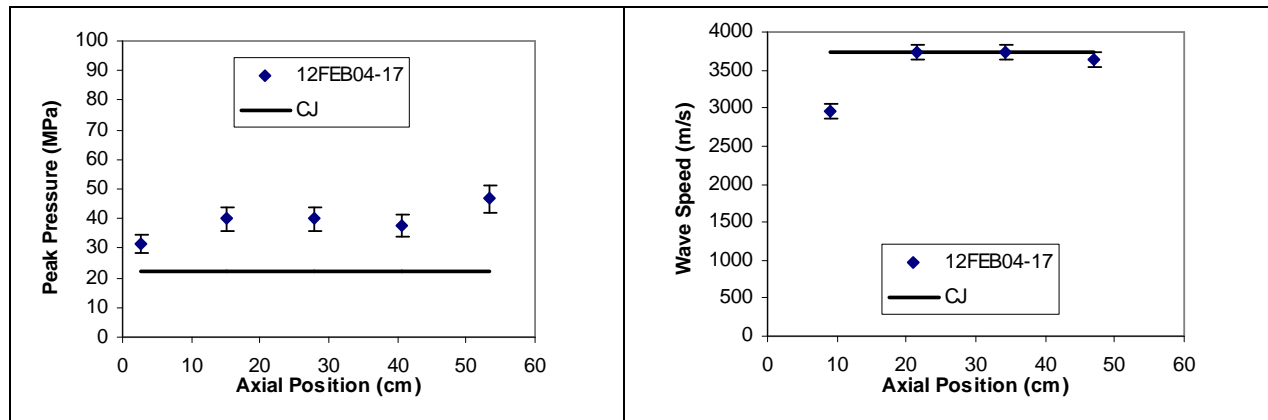
Detonations of cryogenic mixtures of gaseous-hydrogen and liquid-oxygen were found to be characterized by higher than CJ propagation velocities as well as high average and fluctuating wall pressures. These results differ from those obtained by other researchers for cryogenic gaseous-hydrogen gaseous-oxygen mixtures and ambient temperature spray detonations as discussed previously. Explanations for the new findings were sought in the fact that the apparatus used in this study was designed to represent conditions that are expected to be significant to the design of a PDRE; i.e., relative to previous studies, the tube was short and the mixtures were flowing and non-uniform.

### B. Transient Effects

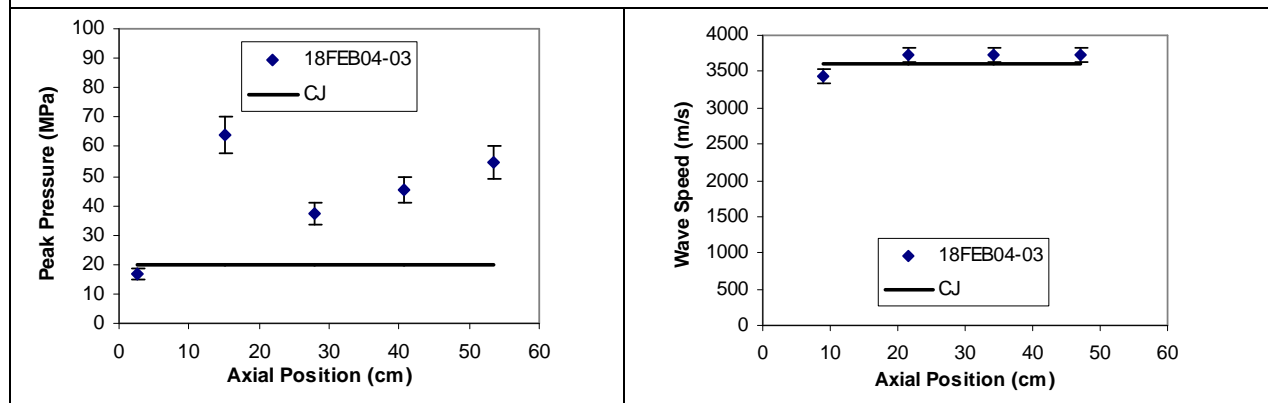
Scientific detonation studies are usually performed in tubes several meters long to ensure that steady state conditions have been reached at the measurement location. The distance required depends on the method of initiation and the initial density, but generally a detonation passes through an over-driven condition before relaxing to a steady velocity<sup>4</sup>. While in the over-driven state the detonation propagates at a higher velocity and has higher peak pressure than CJ values. Thus a transient effect appears to be a plausible explanation for the observations.

**Table 1. Initial conditions for two tests with cryogenic mixtures at high equivalence ratio. Tests represent injector-end and exit-end ignition locations. The liquid oxygen was vaporized at the exit of the tube.**

	12FEB04-17	+/-	18FEB04-03	+/-
Equivalence ratio, $\Phi$	2.44	0.15	2.07	0.13
LOX injector temp. TC04 (K)	120.9	0.6	119.8	0.6
Hydrogen inlet temp. TC10 (K)	122.9	0.6	106.6	0.6
Upper wall temp. TC07 (K)	112.9	1.1	107.4	1.1
Lower wall temp. TC09 (K)	118.6	1.1	107.8	1.1
Exit mixture temp. TC08 (K)	105.3	0.56	90.7	0.56
Initial tube press. PT06 (Pa)	430711	8623	360576	8623
Mixture density (Kg/m <sup>3</sup> )	3.52	0.28	3.77	0.32
Initial gaseous O <sub>2</sub> fraction	0.88	0.04	0.60	0.02
Exit gaseous O <sub>2</sub> fraction	1.00	0.00	1.00	0.00
Mixture average velocity (m/s)	33.7	3.1	30.1	3.0
Ignition location	Exit		Injector	
Theoretical CJ velocity (m/s)	3727		3619	
Theoretical CJ pressure (MPa)	22.3		19.91	



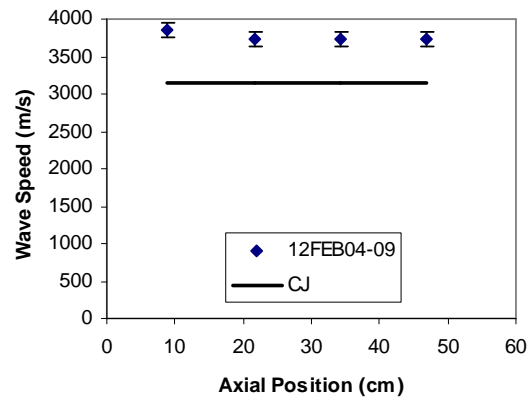
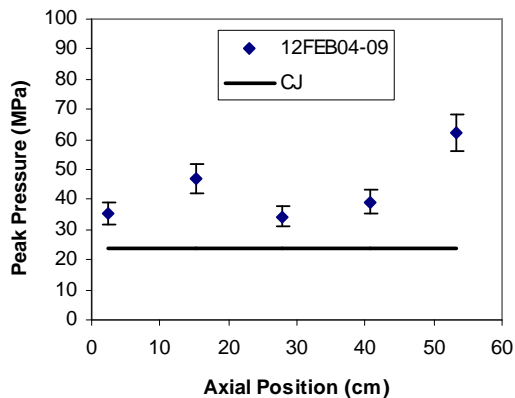
**Figures 5 and 6. Data for high equivalence ratio cryogenic detonation ignited at exit of tube. Oxygen was partially vaporized near injector and fully vaporized at exit. Detonation propagates at near CJ velocity and with wall pressures relative to CJ similar to those obtained in ambient temperature test.**



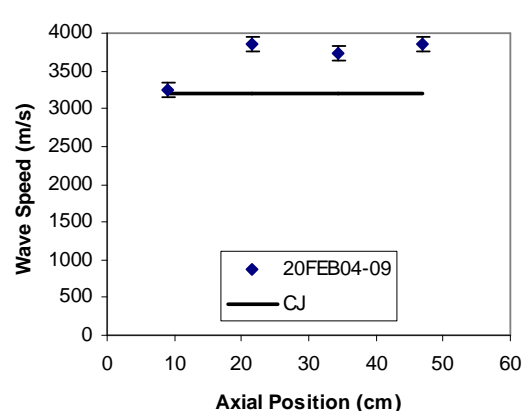
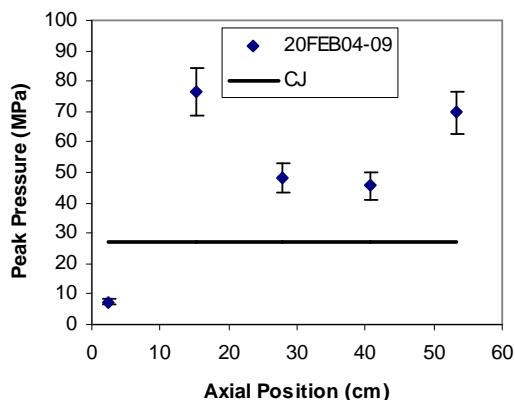
**Figures 7 and 8. Data for high equivalence ratio cryogenic detonation ignited near injector. A higher fraction of oxygen was in a liquid state than the previous test (12FEB04-17). The oxygen was fully vaporized at the exit. Wall pressures are significantly higher than CJ and wave velocities slightly higher relative to results obtained for ambient temperature test.**

**Table 2. Initial conditions for two tests with cryogenic mixtures at near-unity equivalence ratio. Tests represent injector-end and exit-end ignition locations.**

	12FEB04-09	+/-	20FEB04-09	+/-
Equivalence ratio, $\Phi$	1.15	0.05	1.18	0.05
LOX injector temp. TC04 (K)	105.6	0.6	101.7	0.6
Hydrogen inlet temp. TC10 (K)	117.9	0.6	111.3	0.6
Upper wall temp. TC07 (K)	112.4	1.1	106.0	1.1
Lower wall temp. TC09 (K)	113.6	1.1	105.6	1.1
Exit mixture temp. TC08 (K)	107.4	0.6	102.3	0.6
Initial tube press. PT06 (Pa)	409959	8623	430200	3446
Mixture density (Kg/m <sup>3</sup> )	5.12	0.31	5.56	0.30
Initial gaseous O <sub>2</sub> fraction	0.40	0.01	0.34	0.01
Exit gaseous O <sub>2</sub> fraction	1.00	0.00	1.00	0.00
Mixture average velocity (m/s)	33.5	2.4	34.0	2.1
Ignition location	Exit		Injector	
Theoretical CJ velocity (m/s)	3152		3208	
Theoretical CJ pressure (MPa)	23.7		27.08	



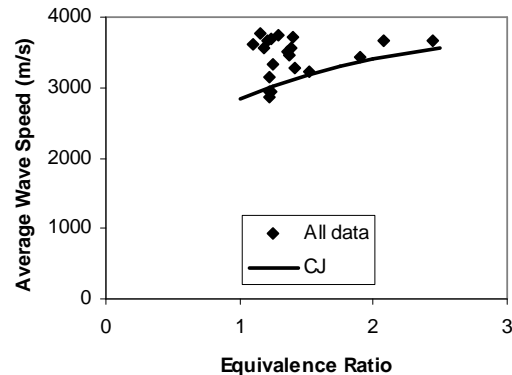
**Figures 9 and 10. Data for low equivalence ratio cryogenic detonation ignited at the exit. Oxygen was estimated to be 66% liquid after injection and nearly vaporized at the exit. Both wall pressures and wave speeds are significantly greater relative to CJ than results obtained in ambient temperature test.**



**Figures 11 and 12. Data for low equivalence ratio cryogenic detonation ignited near the injector. Oxygen was estimated to be 66% liquid after injection and nearly vaporized at the exit. Both wall pressures and wave speeds are significantly greater relative to CJ than results obtained in ambient temperature test. Wall pressures exhibit large fluctuations.**



Previous studies of cryogenic and high pressure hydrogen-oxygen detonations did not report the minimum distance required to reach steady conditions; however in one study<sup>3</sup>, reasonably good agreement with the CJ state was obtained in less than 10 cm. In addition, data obtained in this study includes instances where the detonation accelerated after the wave was fully formed. There were also instances where the wall pressure decreased at the same time the velocity increased. These observations were not consistent with the hypothesis that the detonations were over-driven due to an initiation transient.



**Figure 13. All wave speed results plotted as a function of equivalence ratio. CJ theory represents a lower bound on the data.**

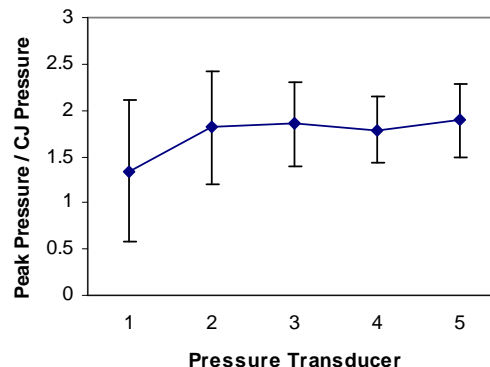
### C. Non-uniform Mixtures

The mixtures in the tube were non-uniform in the axial direction due to vaporization and heat addition from the tube, and also in the radial direction because the hollow-cone spray directed liquid oxygen onto the wall. Due to the large density difference between the oxygen-rich wall layer and the hydrogen, the radial stratification likely persisted for many diameters downstream of the injector. This may have created a situation similar to that reported for solid explosives with gas-filled longitudinal channels<sup>9</sup>. In those systems, the explosion products act as a piston on the gas, driving a powerful shock down the channel, which in turn initiates or accelerates the reaction in the solid. Detonations have been observed to propagate at 1.5-2 times the velocity of the solid charge alone. There has been some previous work on layered detonations in gaseous systems; however, high-speed detonations have not been reported. Dabora<sup>10</sup> et al. found that surrounding a gaseous detonation with a layer of inert gas in fact causes a velocity decrement that depends on the density ratio of the reactive gas to the inert, and the width of the reactive layer. When hydrogen or helium was used in the inert layer, the reaction zone was observed to propagate at 50% of the CJ velocity. The studies of layered mixtures of Liu<sup>11</sup> and Jones<sup>12</sup> also did not report higher than CJ velocities and pressures, apparently because these studies focused on diffraction phenomena during the initial formation of the detonation in the surrounding layer.

### D. Numerical Simulations

Numerical simulations were performed to test the layered detonation hypothesis using CFD++, a commercially available code from Metacomp Technologies for compressible reacting flows. Only the overall features of the flow were of interest, so the simulations were performed with a mesh size set at approximately 10 times the estimated detonation cell size, or 0.41 mm in the axial direction and 0.67 mm in the radial. Hydrogen-oxygen chemistry was modeled using a 9 species, 18 reactions mechanism. An inviscid Euler equation set was solved using a scheme second order accurate in global time step.

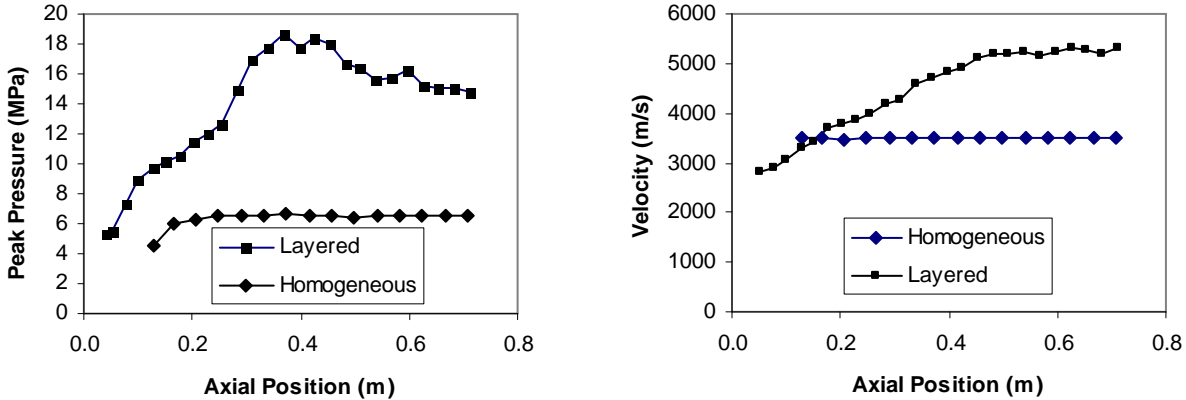
For the layered detonation simulation, half of the cross-sectional area adjacent to the wall was filled with a stoichiometric mixture of hydrogen and oxygen, and the other half along the centerline was filled with hydrogen. A second simulation was performed as a control where the same amounts of reactants were distributed uniformly across the tube for an equivalence ratio of 2.5. In both cases the initial pressure was 1 atmosphere and the temperature was 100 K. The detonations were initiated by a 2.5 cm



**Figure 14. Peak wall pressures average nearly a factor of two greater than CJ theory. Large fluctuations are typical.**

layer adjacent to the closed end of the tube that was initialized at 10 atm and 1800 K.

Results for wave speed and peak wall pressure as a function of axial distance along the tube are given in figure 15. The detonation in the layered mixture initially propagates at the CJ velocity of the stoichiometric layer but then accelerates from 2800 m/s to 5300 m/s, while the detonation in the uniform mixture propagates at a steady velocity of 3500 m/s. The peak wall pressure of the layered detonation is initially at the CJ detonation pressure of the stoichiometric layer but then increases to a maximum of three times that of the homogeneous mixture and then decreases to a steady value approximately 2.5 times the homogeneous. In summary, the calculations exhibit the same qualitative characteristics observed in the experiments: high velocities and peak wall pressures and large changes in velocities and pressures.



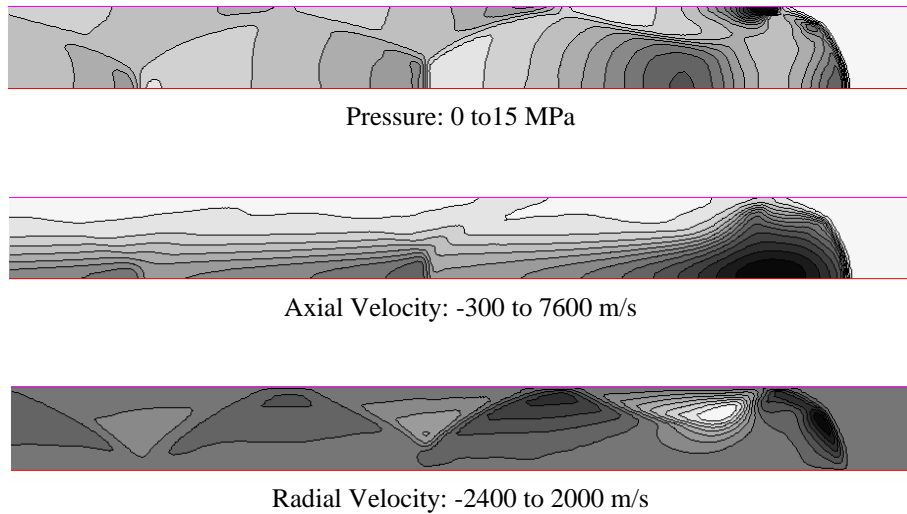
**Figures 15 and 16. Results of CFD simulations of detonation in a layered mixture of stoichiometric hydrogen and oxygen in wall layer and hydrogen on centerline. Wave velocities and wall pressures exceed the values obtained for a homogeneous mixture of the same components.**

#### E. Layered Detonation Flow Features

Figure 16 shows some of the key features of the layered detonations. The leading shock in the hydrogen layer along the centerline is curved. There is a break in the curve at the boundary between hydrogen and hydrogen/oxygen wall layer. In the wall layer the shock is highly oblique (approximately  $20^\circ$  angle to the direction of incoming flow). The shock strength is insufficient to initiate prompt reactions and propagate as an oblique detonation; instead the reaction zone is concentrated at the point where the oblique shock reflects from the wall. Due to the compression by the incident and reflected shocks, peak pressure in this zone is 15 MPa or 2.5 times the CJ detonation pressure of a homogeneous mixture.

Expansion waves emanating from the reaction zone compress the core hydrogen and create a high pressure region on the axis about 1 tube diameter behind the shock front. The pressure drives a flow of hydrogen along the axis at 7600 m/s in the direction of travel of the detonation. This flow recompresses and drives the leading shock front.

The reaction zone sets up transverse waves that couple with the tube and persist for many tube diameters behind the front. These waves are unrelated to any detonation cell structure which would exist at length scales an order of magnitude below the resolution of the simulation; in fact, due to the fundamentally different mode of propagation, detonation cell structure as it is commonly understood may not exist for this mode of propagation. Since the reaction zone is concentrated at the point the oblique shock reflects from the wall, there may not be any propagating Mach-stems traversing the wave front.



**Figure 16. Pressure (top), axial-velocity (middle), radial-velocity (bottom) for layered detonation of stoichiometric gaseous hydrogen and oxygen in wall layer and hydrogen along centerline. Magnitude increases as grey scale darkens. Wave is moving left to right. Wall is at top and centerline at bottom. Initial state is 1 atm and 100 K.**

#### **F. Specific Impulse**

An interesting question relevant to pulse detonation rocket engines is whether the high propagation velocity and wall pressure of a detonation in a layered mixture of hydrogen and oxygen could result in an increase in specific impulse relative to a homogeneous mixture. Included in the simulations was a calculation of the impulse produced from the time of ignition until the tube pressure equaled the ambient pressure. The exit flow was modeled by including the region 1 meter axially and 0.75 meter radially from the exit. This region was initialized with 100 Pa of hydrogen. The exit boundary condition for the tube was initially specified to be a one-way flow blockage boundary. When the detonation front reached the exit, the boundary condition was changed to an exit flow boundary condition.

The layered detonation produced an impulse of 0.870 N-s and the homogeneous 0.907 N-s. We attribute the lower impulse of the layered detonation to higher dissociation in the stoichiometric layer and the divergence angle of the exit flow.

### **V. Conclusion**

Detonations in cryogenic gaseous-hydrogen/liquid-oxygen mixtures were observed to propagate at velocities up to 20% higher and produce wall pressures up to a factor of 3 higher than Chapman-Jouget equilibrium code calculations. This behavior differed significantly from previous studies of cryogenic gaseous-hydrogen, gaseous-oxygen detonations which exhibited close agreement with CJ calculations, and also differed from previous studies of detonations in sprays which exhibited lower than CJ velocities and pressures. Consideration of the data in several cases leads us to believe that this was not a transient phenomena associated with an initially overdriven detonation relaxing to a steady state.

In this study the liquid oxygen was sprayed into the chamber in a hollow-cone pattern that directed the liquid onto the wall of the tube. This created a layered mixture that had a high concentration of oxygen on the periphery and a low concentration on the centerline. CFD calculations showed that detonations in mixtures configured in this way can propagate at velocities a factor of 2 higher, and produce peak wall pressures up to a factor of 3 higher than the CJ values of homogeneous mixtures.

The layered detonation phenomena does not appear to have any advantages for pulse detonation rocket engines as the theoretical impulse was 96% of that of a homogeneous mixture at the same initial state.

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